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THE EVALUATION OF QUANTUM INTEGRALS

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The application of the Wilson-Sommerfeld quantum conditions to a conditionally periodic system with orthogonal coördinates involves the evaluation of an integral of the type

$$J = \oint \sqrt{f(q)} dq. \quad (1)$$

The integral is to be extended over a complete cycle of values of q , which oscillates between two roots of $f(q)$. The sign of the radical is to be the same as that of dq , so that if a and b denote the roots of $f(q)$, the integral can be written

$$J = 2 \int_a^b \sqrt{f(q)} dq \quad (2)$$

If $f(q)$ is a polynomial of the second degree in either q or $1/q$ the integral can be cleanly evaluated. Otherwise, approximations are generally necessary. If $f(q)$ can be expressed in the form

$$f(q) = \varphi(q) + \alpha \psi(q)$$

where $\varphi(q)$ is quadratic in q or $1/q$, α is constant, and $\alpha\psi(q)$ is small, a natural method of procedure is to try to develop J into a power series in α . Thus

$$J(\alpha) = J(0) + \alpha J'(0) + \frac{\alpha^2 J''(0)}{2!} + \frac{\alpha^3 J'''(0)}{3!} + \dots \quad (3)$$

$J(0)$ and $J'(0)$ are easily evaluated, but unfortunately the higher derivatives of J with respect to α cannot be calculated by the usual methods because the higher derivatives of $\sqrt{f(q)}$ with respect to α become infinite at $q = a$ and $q = b$. Hence this method is useful only when the higher order terms are negligible.¹

Another method of attack employed by F. Tank² and accepted as valid by others³ turns out on close examination to be faulty. Tank de-

velops $f(q)$ into a power series about its maximum point, $q = d$. Let $\xi = q - d$, and let H denote the maximum value of $f(q)$. Then $f(q)$ can be thrown into the form

$$f(q) = H - \alpha\xi^2 - (\beta\xi^3 + \gamma\xi^4 + \delta\xi^5 + \dots). \quad (4)$$

Introducing the symbols

$$\begin{aligned} V(\xi) &= \alpha\xi^2, \\ \Delta V &= \beta\xi^3 + \gamma\xi^4 + \delta\xi^5 + \dots, \end{aligned}$$

we obtain

$$\sqrt{f(q)} = \sqrt{H-V} \sqrt{1 - \frac{\Delta V}{H-V}} = \sqrt{H-V} - \frac{1}{2} \frac{\Delta V}{\sqrt{H-V}} - \frac{1}{8} \frac{(\Delta V)^2}{\sqrt{(H-V)^3}} - \dots$$

Tank in effect integrates this series term by term between the limits $-(H/\alpha)^{1/2}$ and $+(H/\alpha)^{1/2}$ and identifies twice the sum of the series so obtained with J . This procedure is wrong, since the correct limits of integration for J are $\xi = a - d$ and $\xi = b - d$. Moreover, the expansion is not usually convergent throughout the interval of integration, so that it is not possible to correct Tank's work by altering the limits.

Another scheme of series development may be suggested, which avoids the above difficulty. Let the quantity u be defined by the equation

$$H = \sqrt{H - f(q)} = \xi \sqrt{\alpha + \beta\xi + \gamma\xi^2 + \delta\xi^3 + \dots}. \quad (5)$$

The sign of u is to be the same as that of ξ . The integral J can now be thrown into the form

$$\begin{aligned} u &= +\sqrt{H} \\ J &= 2 \int_{-\sqrt{H}}^{+\sqrt{H}} \sqrt{H-u^2} \frac{d\xi}{du} du \\ u &= -\sqrt{H} \end{aligned} \quad (6)$$

Let us assume that $d\xi/du$ can be developed into a power series in u . Thus

$$\frac{d\xi}{du} = \sum_{\tau=0}^{\infty} a_{\tau} u^{\tau} \quad (7)$$

Let

$$K_{\tau} = 2 \int_{-\sqrt{H}}^{+\sqrt{H}} u^{\tau} \sqrt{H-u^2} du. \quad (8)$$

To evaluate K_{τ} we introduce the variable of integration θ defined by the relation $u = H^{1/2} \sin \theta$.

Then (8) becomes

$$K_{\tau} = H^{\frac{\tau+2}{2}} \int_0^2 \sin^{\tau} \theta \cos^2 \theta d\theta. \quad (9)$$

It is easy to show from (9) by the application of well-known formulae that K_τ vanishes for odd values of τ ; that K_0 is πH ; and that for even values of τ greater than zero K_τ is given by the equation

$$K_\tau = 2\pi H^{\frac{\tau+2}{2}} \varphi(\tau) \quad (10)$$

where

$$\varphi(\tau) = \frac{1.3.5 \dots (\tau-1)}{2.4.6 \dots (\tau+2)}. \quad (11)$$

Now (6) becomes

$$J = \pi H [a_0 + 2 \sum_{\tau=1}^{\infty} a_{2\tau} \varphi(2\tau) H^\tau]. \quad (12)$$

We proceed to the evaluation of the coefficients a_0, a_1, a_2, \dots . As $d\xi/du$ may be regarded as a function of either ξ or u , let

$$d\xi/du = \psi(u) = \chi(\xi).$$

Then

$$a_\tau = \frac{1}{\tau!} \psi^{(\tau)}(0). \quad (13)$$

Since u and ξ vanish together, the derivatives of ψ at the point $u = 0$ can be calculated from the derivatives of χ at the point $\xi = 0$. The following method of procedure is perhaps the simplest. Let

$$v(\xi) = \frac{H-f(q)}{\xi^2} = \alpha + \beta\xi + \gamma\xi^2 + \dots \quad (14)$$

Then $u = \xi^{-1/2}$ and $\frac{du}{d\xi} = \frac{v + \frac{1}{2}\xi v'}{\sqrt{v}}.$

Let $w = 2v(\xi) + \xi v'(\xi) = -\frac{f'(\xi+d)}{\xi}.$ (14')

Then $\chi(\xi) = \frac{1}{\frac{du}{d\xi}} = \frac{2\sqrt{v(\xi)}}{w(\xi)}.$ (15)

Differentiating,

$$\left. \begin{aligned} \psi'(u) &= \chi'(\xi) \chi(\xi) \\ \dots &= \dots \\ \psi^{(n)}(u) &= \chi(\xi) \frac{d}{d\xi} \left\{ \psi^{(n-1)}(u) \right\} \\ \dots &= \dots \end{aligned} \right\} \quad (16)$$

In some cases these successive derivatives of ψ are simple and easily calculated functions of ξ . In others the successive derivatives rapidly become complicated. If $f(q)$ is given as a power series in ξ the process of differentiation can be performed conveniently as follows:

$$\left. \begin{aligned}
 \psi'(u) &= \frac{2v'}{w^2} - \frac{4vw'}{w^3}, \\
 \psi''(u) &= \frac{4\sqrt{v}}{w^3} \left\{ v'' - \frac{4v'w'}{w} - \frac{2vw''}{w} + \frac{6v(w')^2}{w^2} \right\} \\
 \psi'''(u) &= \frac{4}{w^4} \left\{ v'v'' + 2vv'' - \frac{14vv''w'}{w} - \frac{4(v')^2w''}{w} - \frac{14v'v''w''}{w} \right. \\
 &\quad \left. + \frac{50vv'(w')^2}{w^2} + \frac{40v^2w'v''}{w^2} - \frac{4v^2w'''}{w^2} - \frac{60v^2(w')^3}{w^3} \right\}
 \end{aligned} \right\} (17)$$

At the point

$$\left. \begin{aligned}
 u &= \xi = 0, \\
 w &= 2v = 2\alpha, & w' &= 3v' = 3\beta \\
 w'' &= 4v'' = 8\gamma & & \\
 w^{(n)} &= (n+2)v^{(n)} = \dots
 \end{aligned} \right\} (18)$$

Hence

$$\left. \begin{aligned}
 \psi(0) &= \frac{1}{\sqrt{\alpha}} \\
 \psi''(0) &= \frac{3}{\alpha^{5/2}} \left\{ \frac{5}{4} \frac{\beta^2}{\alpha} - \gamma \right\}, \\
 \psi^{IV}(0) &= \frac{105}{\alpha^{7/2}} \left\{ \frac{33}{16} \frac{\beta^4}{\alpha^3} - \frac{9}{2} \frac{\beta^2\gamma}{\alpha^2} + \frac{2\beta\delta}{\alpha} + \frac{\gamma^2}{\alpha} - \frac{4}{7} \epsilon \right\}.
 \end{aligned} \right\} (19)$$

Combining the above equations with (13), (11), and (12), we obtain

$$\begin{aligned}
 J &= \pi \psi(0)H + 2\pi \varphi(2) \frac{\psi''(0)}{2!} H^2 + 24 \varphi(4) \frac{\psi^{IV}(0)}{4!} H^3 + \dots \\
 &= \frac{\pi H}{\sqrt{\alpha}} \left\{ 1 + \frac{3}{8\alpha^2} \left[\frac{5}{4} \frac{\beta^2}{\alpha} - \gamma \right] H + \frac{35}{64\alpha^3} \left[\frac{33\beta^4}{16\alpha^3} - \frac{9}{2} \frac{\beta^2\gamma}{\alpha^2} \right. \right. \\
 &\quad \left. \left. + \frac{2\beta\delta}{\alpha} + \frac{\gamma^2}{\alpha} - \frac{4}{7} \epsilon \right] H^2 + \dots \right\}.
 \end{aligned} \quad (20)$$

This result is similar in form to Tank's and the coefficients of the two lowest powers of H are the same as in his series, but the coefficient of H^3 is different.

In order that the result may be valid, it is necessary that the series (4) converge and represent $f(q)$ throughout the interval of integration, and that the derivatives of ψ shall all be finite throughout a circle whose radius is greater than $+H^{1/2}$ drawn about the origin on the complex u plane. From (17) it is evident that the derivatives of ψ will be finite up to the point where w vanishes. It follows from (14') that $f'(q)/(q-d)$ must have no zeros on that part of the complex q plane which is mapped on the above-mentioned circle on the u plane. It is necessary, in particular, that $f'(q)$ shall vanish not more than once for real values of q between a and b .

It does not seem worth while to attempt an exact discussion of the boundaries of the region on the complex q plane from which the zeros of $f'(q)/(q-d)$ must be excluded, but we can say qualitatively that there is little chance that the series (7) will not converge throughout the interval of integration if the series

$$w = 2\alpha + 3\beta\xi + 4\gamma\xi^2 + 5\delta\xi^3 + \dots \quad (21)$$

converges rapidly.

In the applications of this analysis an expression for H as a function of J will generally be desired. The power series may be reversed to advantage by the following scheme which resembles that of Lagrange. Let $H = F(J)$. Then by Taylor's theorem

$$H = JF'(O) + \frac{J^2}{2!}F''(O) + \frac{J^3}{3!}F'''(O) + \dots \quad (22)$$

Let b_n denote the coefficient of H^n in (20). $F'(O)$, $F''(O)$, etc., can be calculated in terms of the b 's. Let us first compute the derivatives of F in terms of H . Let

$$p(H) = \sum_{n=1}^{\infty} nb_n H^{n-1} = \frac{dJ}{dH}.$$

Then

$$\frac{dH}{dJ} = F'(J) = \frac{1}{p(H)}. \quad (23)$$

Differentiating again,

$$\left. \begin{aligned} F''(J) &= \frac{d}{dH} \left(\frac{1}{p} \right) \cdot \frac{dH}{dJ} = -\frac{p'}{p^3} \\ F'''(J) &= \frac{d}{dH} \left(-\frac{p'}{p^3} \right) \frac{dH}{dJ} = -\frac{p''}{p^4} + \frac{3(p')^2}{p^5} \\ &\dots \dots \dots \end{aligned} \right\} \quad (24)$$

Since J vanishes when H does, the values of $F'(O)$, $F''(O)$, etc., are obtained by setting H equal to zero in the right-hand members of (23) and (24). Thus

$$\left. \begin{aligned} F'(O) &= 1/b_1; & F''(O) &= -2b_2/b_1^3; \\ F'''(O) &= -6b_3/b_1^4 + 12b_2^2/b_1^5; \\ &\dots \dots \dots \end{aligned} \right\} \quad (25)$$

If these formulas for $F'(O)$, $F''(O)$, etc., are evaluated in terms of the expressions for the b 's given by (20), equation (22) becomes

$$H = \frac{\sqrt{\alpha}}{\pi} J + \frac{3}{8\pi^2\alpha} \left[\gamma - \frac{5\beta^2}{4\alpha} \right] J^2 + \frac{1}{32\pi^3\alpha^{3/2}} \left[10\epsilon - \frac{35\beta\delta}{\alpha} \right] J^3 + \dots$$

$$-\frac{17}{2} \frac{\gamma^2}{\alpha} + \frac{225}{4} \frac{\beta^2 \gamma}{\alpha^2} - \frac{705}{32} \frac{\beta^4}{\alpha^3} \Big] J^3 + \dots \quad (26)$$

As a check on the series development here suggested, the writer has derived Sommerfeld's formula,

$$\oint \sqrt{A + \frac{2B}{q} + \frac{C}{q^2}} dq = 2\pi \sqrt{-C} \left[\frac{B}{\sqrt{AC}} - 1 \right] \quad (27)$$

by means of the series (12). The derivatives of ψ when evaluated by equations (16) are in this case particularly simple and as a result the series can be summed.

It is of interest to note that the method of development in series here suggested is applicable to a variety of problems. It may be used to evaluate indefinite as well as definite integrals.

One simple application is in the determination of the periods of oscillation of a vibrating system. In the case of a conditionally periodic system with orthogonal coordinates, the periods are given by expressions of the form

$$T = \oint \frac{dq}{q} = 2 \int_a^b \frac{dq}{a \sqrt{f(q)}}, \quad (28)$$

where a and b are again roots of $f(q)$. Introducing the quantities H , ξ , u defined as in the preceding work, we obtain

$$T = 2 \int_{-\sqrt{H}}^{+\sqrt{H}} \frac{d\xi / du}{\sqrt{H - u^2}} du. \quad (29)$$

If $d\xi/du$ is developed into a power series of the type (7), we obtain

$$T = \sum_{\tau=0}^{\infty} a_{\tau} \bar{K}_{\tau}$$

where

$$\bar{K}_{\tau} = 2 \int_{-\sqrt{H}}^{+\sqrt{H}} \frac{u^{\tau} du}{\sqrt{H - u^2}} = H^{\tau/2} \int_0^{2\pi} \sin^{\tau} \theta d\theta.$$

The coefficients \bar{K}_{τ} vanish when τ is odd, and the final expression for the period is

$$T = 2\pi \left[a_0 + 2 \sum_{\tau=1}^{\infty} a_{2\tau} (\tau+1) \varphi(2\tau) H^{\tau} \right]. \quad (30)$$

¹ This is in effect the method used by Sommerfeld, *Atombau und Spektrallinien*, 2nd edition, Braunschweig, 1921, pp. 476-482.

² F. Tank, *Mitteilungen Physik. Ges. Zurich*, 1919, p. 87.

³ Cf. G. Hettner, *Zs. Physik.*, 1, 4, 1920 (350).